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Delivered Date: 10/06/2006 05:44 PM PST

Subject: RE: LDWG_FWM_Results of Draft Food Web Model runs

Hi everyone. There was one more point I meant to cover in my last e-mail that I overlooked. It's the decision to treat the average sediment concentration (" *baseline SWAC* ") as a point estimate for model calibration. We talked about this in very general terms at the September 12 meeting, and I sensed people were generally comfortable with it then. Here's a more detailed explanation of why it's a good idea. What it boils down to is that the SWAC is a decision variable in the sense of Morgan and Henrion (1990, p. 52):

"Decision variables are quantities over which the decision maker exercises direct control. They are sometimes also referred to as control variables *or* policy variables . *For example, in a risk assessment model designed to help an EPA decision maker set a standard for a particular air pollutant, the permitted maximum ambient level or total quantity of pollutant emitted might be a decision variable. …One may very well be uncertain about the "best" value for a decision variable – otherwise why would we be constructing a policy model in the first place? But it does not make sense to be uncertain about its "true" value. If it is a decision variable, then by definition it has no true value. It is up to the decision maker to select its value."*

We're calibrating the model so that it can be used to predict the "target SWAC" (*RBTC*) associated with a risk-based tissue concentration threshold (TRV). By Morgan and Henrion (1990, pp. 51-53), *RBTC* should be treated parametrically because it is a decision variable. "Treated parametrically" means that the analysis should be repeated with a range of possible values (of *RBTC*) until it produces the desired outcome, i.e., some specific, well defined estimate of tissue concentration = TRV. (The decision about what to use as the "specific, well defined estimate of tissue concentration" hasn't been made yet, but it might, for example, be the expected value of the mean total PCB tissue concentration in a market basket-weighted average of individual species' tissue concentrations.)

If we're treating *RBTC* parametrically when we use the model, then we should treat *baseline SWAC* as a point estimate – not probabilistically – for model calibration. It should be calculated in a manner that's as consistent as possible with the *RBTC* that will be used to calculate AOPCs. So, for example, if LDWG will be using IDW to calculate AOPCs in the FS, then we should calculate both *baseline SWAC* and *RBTC* as the simple average of values on an IDW grid, where both IDW grids are based on the same underlying data set, and differ only in the substitution of replacement values to achieve *RBTC* .

Treating *baseline SWAC* as a point estimate for calibration will produce different calibrated distributions on other FWM parameters than we'd get if we treated *baseline SWAC* probabilistically (because the GSA procedure will select those parameter values that work with the *baseline SWAC* point estimate in predicting mean tissue concentrations within a specified model performance criterion). That's okay, and again it's the right thing to do, because the model will be used with a deterministic *RBTC* (the decision variable) that's calculated in the same manner as the *baseline SWAC* point estimate.

I hope this is clear… and makes sense! Please let me know if you have any questions.

John

Literature cited

Morgan, MG and Henrion, M (with a chapter by Small, M). 1990. *Uncertainty: A Guide to Dealing with Uncertainty in Quantitative Risk and Policy Analysis* . First Edition. Cambridge University Press, Cambridge , UK .

From: John Toll

Sent: Friday, October 06, 2006 3:14 PM

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Subject: RE: LDWG_FWM_Results of Draft Food Web Model runs

Bruce Burt, Jay and Allison,

I'm following up on Fiona's e-mail of yesterday afternoon; I've got some more detail for you about how we're using the information in the tables she sent you yesterday for thinking about calibration options. We are still talking internally about approaches to

calculating risk based tissue concentrations (RBTCs), so I'm going to have to hold off on discussing that probably until we meet on Tuesday.

Fiona sent you three tables. Table 1 just summarizes the prior and posterior distributions on food web model (FWM) parameters, and Table 2 shows what proportion of the possible combinations of parameter values met model performance criteria of different stringencies.

We've filtered FWM output using many difference model performance criteria, but the ones shown in Tables 1 and 2 are based on the constraint that all species predictive accuracy factors (SPAFs) must be less than a threshold value. The thresholds we chose to evaluate were 3, 2 and 1.5. (The meaning of a SPAF of *x* is that FWM-predicted tissue concentration for a species must be within a factor of *x* of the empirical mean tissue concentration for that species.) We think that an "All SPAF" criterion is a reasonable way to go because it considers the model's ability to predict all species' tissue concentrations (i.e., it doesn't ignore the poor performer). The other type of criterion that considers the model's ability to predict all species' tissue concentrations is a mean SWAC-based criterion. That's an option but it seems less satisfactory because it suggests that the model doesn't have to be able to meet the desired performance threshold for all species, just on average. So, we've focused in on "All SPAF" criteria.

The range of 3, 2 and 1.5 is useful because it runs the gambit from a criterion that the model easily meets (All SPAF < 3) to a criterion that the model rarely meets (All SPAF < 1.5). It also covers the range of performance levels people tend to think steady state FWM's can achieve (within a factor of 2-3).

What you see when you look at Table 1 is that filtering probabilistic FWM predictions based on All SPAF < 3 has very little effect on parameter distributions, filtering based on All SPAF < 2 has a somewhat greater effect and filtering based on All SPAF < 1.5 has a fairly severe effect. We think that All SPAF < 1.5 would result in a calibrated model with low predictive power because the range of model predictions will actually be tighter than the uncertainty about site-wide tissue concentrations, i.e., we think that additional empirical data are likely to invalidate such a tightly calibrated model. Using the All SPAF < 3 criterion would more or less amount to saying that the prior probability distributions are more or less okay as is. Using the All SPAF < 2 criterion does start to tighten up parameter ranges, but not to the point that most parameter combinations don't work. Using All SPAF < 1.5 filters out 99.9% of parameter combinations. This seems to argue against using an All SPAF < 1.5 criterion. All SPAF < 2 is an achievable performance threshold, and our analysis so far doesn't lead us to believe that it's posterior distributions are unreasonably tight, so we think it could be a good calibration choice.

As Fiona mentioned Table 3 summarizes model parameters most highly correlated with FWM-predicted tissue concentrations. This particular table is for the All SPAF < 2 criterion. We have tables like this for the other model performance criteria as well but chose to focus on this one because we consider it our best option at this point. The correlated parameter table is useful because it gives a sense of which parameter uncertainties most affect model predictions. You'll see from Table 3 that what seem most important (in this sense) are a) FWM assumptions about organisms' lipid content, b) whether consumers are eating zooplankton or benthic invertebrates, and c) water column PCB concentration. We're still looking at input-output correlations and also correlations between FWM parameters. How far we pursue that will depend on what decisions get made about how to calculate RBTCs. We'll talk about that more on Tuesday, but the general question is whether the group chooses to go with a) fully probabilistic RBTCs, or b) single-valued best estimates of RBTCs with ranges attached. Option (b) is considerably simpler to implement (and perhaps to understand), and doesn't require a lot of information about correlation structure, so if it's selected we'll spend less effort on that, and move straight into the nuts and bolts of model application (RBTC calculation methods).

I hope this is helpful to you as you look at the tables we've provided in advance of Tuesday's meeting. Please let me know if you have questions, comments or concerns. You can e-mail or call between now and Tuesday's meeting or we can take up your questions when we meet. Have a nice weekend,

John

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Sent: Thursday, October 05, 2006 5:18 PM

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Subject: LDWG_FWM_Results of Draft Food Web Model runs

Bruce, Burt, Jay and Alison,

Attached are a few tables summarizing the results of our Monte carol model runs processed through a generalized sensitivity analysis.

Table 1 summarizes the initial probability distributions entered into the Monte Carlo (min, max and mean/mode are presented) and the new min, max and means ("posterior distributions") depending on what SPAF criteria were applied (<SPAF of 3, < SPAF of 2 or < SPAF of 1.5).

This table gives you an idea of how "compressed" or reduced your input distributions become the more stringent your model evaluation criteria become.

(NOTE: "posterior" distributions refers to the values which remained for a parameter once the 20,000 runs were filtered through the generalized sensitivity analysis)

Table 2 summarizes the number of runs (and %) that passed (out of 5490) for each SPAF level. 5490 was the number of runs out of 20,000 that passed through the dietary filter.

Table 3 summarizes model parameters most highly correlated with food web model predicted tissue concentrations. This table helps to understand the parameters that most influence tissue concentrations for each species.

Tomorrow morning, John will be sending out a more detailed description of uses for these tables and as well as some proposals for approaches to calculating risk based tissue concentrations, and a summary of some calibration options and pros/cons.

Thank you

Please email or call myself or John with questions.

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